Estimating molecular hydrogen in diffuse interstellar clouds

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Accepted 1988 November 28. Received 1988 November 25; in original form 1988 July 6

Summary. It is shown that good estimates of the column density of molecular hydrogen in diffuse interstellar clouds may be obtained in two ways: from the atomic hydrogen column density combined with \( E(B-V) \); and from optical observations of CH molecules. The latter method is more accurate.

1 Introduction

In many diffuse interstellar clouds most of the hydrogen is in the molecular form \( \text{H}_2 \), which therefore provides almost all the mass. A knowledge of the \( \text{H}_2 \) abundance is required to determine the mass and gas density in the cloud and, in relation to other molecules, to establish the chemical situation there. Comparing atomic abundances with the total hydrogen abundance – atoms plus molecules – gives the atomic depletions, which provide information about the composition of the dust grains, and also leads to a measure of the metallicity of the cloud material, related to its history of nuclear processing and ultimately to the primordial abundances. The purpose of the present paper is to review the available methods for observing or estimating the abundance of \( \text{H}_2 \) in diffuse clouds.

Unfortunately, the interstellar sight-lines where \( \text{H}_2 \) has been studied directly are comparatively few in number, and this is likely to remain the situation for some time. The ultraviolet absorption lines have wavelengths shortward of 1108 Å, too short to be observed with the IUE satellite. At present, results are available for only just over 100 stars observed with Copernicus (Savage et al. 1977; Bohlin et al. 1983); these stars are relatively bright and many of them have low interstellar reddening. This spectral range will be covered by both the Hubble Space Telescope and the proposed ultraviolet satellite Lyman (Wilson 1986; Linsky 1986), but it seems unlikely that in either case high priority would be given to a general survey of \( \text{H}_2 \) in the directions of large numbers of galactic stars brighter than magnitude \( V \sim 10 \), which is what is required to compare with optical and IUE observations of other species.

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Vibrational emission lines of H$_2$ in the near infrared have been observed (Shull & Beckwith 1982), but they require fairly high excitation temperatures and, being electric quadrupole transitions, they are intrinsically weak. These lines can therefore be observed in emission only from nearby warm clouds and not from the general cold diffuse clouds. The quadrupole pure rotational spectrum of H$_2$, in particular the J = 2–0 line at 28 μm, may also be expected to be observed in emission from warm clouds. H$_2$ has also a very-low-energy structure that comes from the interaction of the two nuclear spins with the nuclear rotation (Somerville 1977); this gives rise to low-frequency radio spectral lines that will be emitted from cold clouds. Field, Somerville & Dressler (1966) called this an ultrafine structure (a more euphonious name than the hyperfine introduced by Tatum 1986, for similar structure in other molecules). The line at 546 kHz, which might on occasion penetrate the ionosphere and reach the ground, has on a very rough estimate a transition probability $A \sim 10^{-28}$ s$^{-1}$; under the most optimistic assumptions, this could give a detectable signal from some nearby giant molecular cloud. However, at this frequency the background continuum from galactic sources is very strong; the signal in this line relative to the continuum would be approximately 1 part in $10^{11}$, so it would require impossibly long exposure times for the line to be observed above the random noise level (A. E. Wright, private communication).

Several indirect methods have been used to estimate the H$_2$ abundance in interstellar clouds. For dense clouds, the microwave emission from CO is used, generally with the assumption that the ratio of N(H$_2$) to the intensity in the CO J = 1–0 line is constant (van Dishoeck & Black 1987). It is accepted that this is a poor assumption, partly because of the uncertain metallicity in these clouds but mainly through the formation there of CO ice on grain mantles (Léger 1983; Whittet, Longmore & McFadzean 1985), the amount of which may differ from cloud to cloud. Solomon et al. (1987) have found a non-linear relation between CO luminosity and virial mass in dense clouds, which has serious implications for studies of cloud stability (Fleck 1988). Direct evidence that a linear relation between CO and H$_2$ does not hold for diffuse clouds comes from the slope in the correlation diagram of Fig. 1, which relates column densities of H$_2$ and CO, both derived from ultraviolet absorption lines. In diffuse clouds, the CO ultraviolet and mm-wave column densities generally are in good agreement (Dickman et al. 1983). In the diffuse clouds of Fig. 1, the column density of CO is proportional approximately to the square of the column density of H$_2$.

Positive molecular ions of hydrogen are expected to be present in the interstellar clouds. The diatomic ion H$_2^+$ is formed by the cosmic ray ionization of H$_2$, and destroyed through collision with H$_2$ to form H$_3^+$, so its abundance is essentially independent of the H$_2$ density in a cloud. It is, however, of interest for its own sake and its role in the cloud chemistry. It is expected that H$_2^+$ will form preferentially in excited vibrational states (Somerville 1977), but a deep search by Shuter et al. (1986) failed to detect the radio-frequency hyperfine-structure transitions in these states, a result that is indeed consistent with the H$_2^+$ abundance predicted by chemical models. This result has been confirmed by more recent observations of still greater sensitivity (Shuter, private communication). The triatomic ion H$_3^+$ is formed from H$_2$ and destroyed by electron impact, so its abundance should reflect that of H$_2$. It may be possible to detect it through observation of its forbidden rotational lines (Pan & Oka 1986), but this emission is likely to be detectable only from a small number of warm interstellar clouds.

The use of atomic abundances to obtain estimates of H$_2$ in diffuse clouds has been suggested. For one star, McLachlan & Nandy (1984) used the Na i D-lines, with a relation based on results of Federman (1981). However, Na i is in general a very minor stage of ionization in diffuse clouds, and the relation between the sodium ionization equilibrium and the hydrogen dissociation equilibrium is not simple. Sodium also generally is depleted onto the grains in these clouds. It is evident from Federman's fig. 2 that there is a very large scatter.
around the relation used by McLachlan & Nandy, so it cannot be expected to give accurate values. Any atomic species that is everywhere undepleted could in principle be used to estimate the hydrogen abundance and to study the depletions of other atoms. It has become clear, however, that no atom is everywhere undepleted. For a time, zinc seemed the best candidate (Harris, Bromage & Blades 1983), using the ultraviolet Zn II doublet, but it has more recently been found that it too suffers depletion as a function of cloud density (Harris & Mas Hesse 1986).

From the Copernicus data, a relation is found between the hydrogen abundance and the amount of dust, expressed through \( E(B-V) \). The correlation has less scatter if the total column density \( N(H) + 2N(H_2) \) is used, rather than atomic hydrogen alone (Bohlin, Savage & Drake 1978). With this relation, \( E(B-V) \) may be used to estimate the amount of hydrogen present; generally, the method has been to estimate the amount of \( H_2 \) with the assumption that atomic hydrogen may be neglected (Crutcher, 1985). Now, there is a clear division in the Copernicus data between sight-lines of low \( H_2 \) and high \( H_2 \) abundance, with few in between – but the change-over does not happen at a unique \( E(B-V) \), for it depends on the cloud volume density as well as the column density. In all the Copernicus sight-lines of high \( H_2 \) abundance, the column densities of atomic and molecular hydrogen are comparable, and for a given \( E(B-V) \) the relative abundances show a significant spread. This spread can be expected to continue to sight-lines of substantially greater reddening. The assumption that atomic hydrogen may be neglected must therefore be applied with some caution. In a more sophisticated application of the same method, Cardelli & Wallerstein (1986) have used \( E(B-V) \) to establish upper and lower limits to \( N(H_2) \).

Two developments lead us to consider new methods for estimating \( H_2 \) abundances that should be more accurate than those used hitherto. The first is the availability from IUE of large datasets of interstellar atomic-hydrogen column densities. Secondly, we are compiling a catalogue of observations of molecules in diffuse clouds (Smith & Somerville, in preparation). From the first draft of the catalogue (Smith, 1987) some clear correlations emerge.
2 Using atomic hydrogen

The Ly-$\alpha$ transition at 1216 Å is easily within the short-wavelength range of IUE. In directions towards reddened stars, the line is heavily saturated and wings produced by radiation damping are clearly present. This gives a simple and unambiguous way to determine the column density (used also for H atoms from Copernicus data), because, in the absence of pressure damping, the intensity in the wing is directly proportional to the column density. Some results have already appeared (Shull & Van Steenberg 1985; Prinjia 1985) and there are many more stars in the IUE archive for which the atomic-hydrogen column density could be obtained.

This suggests that the molecular-hydrogen column density might be estimated from the atomic-hydrogen value and $E(B-V)$, with the relation found for total hydrogen from Copernicus data. This leads to

$$N(H_2) = \frac{1}{2} \left[ 5.8 \times 10^{21} E(B-V) - N(H) \right].$$  \hspace{1cm} (1)

This is the same relation as is given by Bohlin et al. (1978), based here on a sample of 83 stars; stars that they excluded because of uncertain $E(B-V)$ have again been omitted (except for two, for which improved photometry is now available), and we have used also the results of Jenkins, Savage & Spitzer (1986) for the stars they studied. Results obtained using equation (1) may be compared with those from the same correlation formula but assuming that atomic hydrogen may be neglected:

$$N(H_2) = \frac{1}{2} \left[ 5.8 \times 10^{21} E(B-V) \right].$$  \hspace{1cm} (2)

For the Copernicus dataset, equation (1) gives results significantly closer to the true values of $N(H_2)$ than equation (2) does; for the set of 40 stars with $N(H_2)/N(H) > 0.01$, the rms scatter of $N(H_2)$ about the results from equation (1) is $2.3 \times 10^{20}$ cm$^{-2}$, whereas for equation (2) it is $6.0 \times 10^{20}$.

However, for the Copernicus stars more accurate results actually are obtained not from equation (1) which involves the total H$_{tot}$ but from the correlation with $E(B-V)$ of $N(H_2)$ alone:

$$N(H_2) = 5.3 \times 10^{20} E(B-V),$$  \hspace{1cm} (3)

from a sample of 63 stars; for the same subset of 40 stars the rms departure of the measured $N(H_2)$ from this line is $1.0 \times 10^{20}$. Equation (3) gives results closer to the true values than equation (1) does, for 29 stars of the 40 considered. It is more likely to give a poorer value for a more heavily reddened star, for which $N(H_2)$ and $N(H)$ are comparable. As a working rule, in cases where the result of equation (3) is less than 10 per cent of $N(H)$, it is to be preferred to the result of equation (1); in other cases, equation (1) is more likely to give the better result. For the vast majority of stars more heavily reddened than those in the Copernicus dataset (which all have $E(B-V)$ less than 0.5), the value obtained from equation (1) should be better. Thus, for the stars of interest in comparisons with other molecules and other studies using IUE and optical data, equation (1) should be used rather than either of equations (2) or (3).

None of these formulae gives useful results for sight-lines of low molecular column density, $N(H_2) \ll N(H)$.

3 Using molecules

The catalogue of molecules in diffuse clouds (Smith 1987) has been compiled from the column densities given in the original published papers, scaling them where necessary to put them onto the basis of a uniform set of molecular oscillator strengths. In this way, the data from different
observers may be compared directly, although it is recognized that in some cases the use of different data-reduction techniques may introduce scatter. From the data in the catalogue, the column density of molecular hydrogen may be compared with values for other molecules. Results are presented in Table 1, for the three molecules for which we have a reasonable number of points. Consistent with its anomalous column density, which is taken to imply that it is formed in shocks, the correlation coefficient for CH⁺ with H₂ is significantly worse than for the other two molecules. For CH and CO, the correlation coefficients with H₂ are similar and both are large, implying close relationships. However, the value of the correlation coefficient is only part of the story.

Correlation diagrams of CO with H₂ and CH with H₂ are in Figs 1 and 2, respectively. Comparing these diagrams, two differences are apparent. For CH, the data are fitted well by a line of slope 1.0, but for CO the slope is 0.5. These being log-log relations, the CH abundance is thus linearly proportional to the H₂ abundance, but the CO abundance varies as the square of the H₂ abundance — there is relatively more CO in denser clouds. These relations have been noted before (Federman et al. 1980; Danks, Federman & Lambert 1984), with smaller datasets than we have here, and are consistent with chemical models, which indicate that CH is formed

<table>
<thead>
<tr>
<th>Molecule</th>
<th>n</th>
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</tr>
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<tbody>
<tr>
<td>CO</td>
<td>23</td>
<td>0.83</td>
</tr>
<tr>
<td>CH</td>
<td>32</td>
<td>0.82</td>
</tr>
<tr>
<td>CH⁺</td>
<td>38</td>
<td>0.65</td>
</tr>
</tbody>
</table>

\( n \) is the number of points available, using only visible and ultraviolet absorption measures. \( r \) is the correlation coefficient.

**Figure 2.** The correlation of the column densities of CH and H₂. The line has slope 1.0.
directly from H$_2$ and thus is a first-stage molecule in the photochemical processes, whereas CO is formed from OH and so is a second-stage molecule (Federman 1987). Federman & Lambert (1988) have recently introduced N(CH) as the basis of comparison for other molecules in cases where N(H$_2$) is not available. Very recently, de Vries & van Dishoeck (1988) have used the linear relation with N(CH), as well as other methods, to estimate N(H$_2$) in a high-latitude molecular cloud.

The second difference between Figs 1 and 2 is in the amount of scatter about the line, which is substantially more for CO. Apart from observational error, this scatter in the data must come from differences in physical conditions such as cloud density, temperature and optical thickness. Whatever its cause, the scatter gives a measure of the accuracy with which another measurement can be fitted to the line. The closer relation for CH suggests that it is the better one to use for estimating the abundance of H$_2$. Taking the linear relation for CH and the squared relation for CO, which fit the data well, we have

$$N(H_2) = 1.6 \times 10^{13}[N(CO)]^{1/2},$$  \hspace{1cm} (4)

with rms scatter 1.3 $\times$ 10$^{20}$, and

$$N(H_2) = 2.6 \times 10^7 N(CH),$$ \hspace{1cm} (5)

with rms scatter 9.0 $\times$ 10$^{19}$. It is therefore clearly better to use CH rather than CO, for cases where both are observed.

It will be of value to increase the number of points in these comparisons, and to study their validity over a greater range of column densities. More data for CO will come from observations of further *Copernicus* stars already in the IUE archive but not yet published. It is desirable to increase the number of CH observations also, to include the remaining stars with H$_2$ *Copernicus* column densities and particularly to try to observe CH in sight-lines of lower N(H$_2$). The optical CH absorption has the advantage over CO that it can be observed from the ground (mm-wave observations of CO, also ground-based, are not reliable for this purpose because of the possibility of emission from material beyond the star), and can in principle be observed with high spectral resolution. CH has also microwave transitions, the A-doubling transitions at 9 cm. For dense clouds from which these emissions can be observed, it will be worthwhile to use the relation (5), at least to have a check on the results obtained using CO. Mattila (1986) compared radio CH data with the blue extinction A$_B$, and with N(H$_2$) estimated from radio $^{13}$CO observations, and found a continuation of the linear diffuse cloud relationships. However, chemical models of dense clouds suggest that the CH abundance relative to H$_2$ may differ significantly from one cloud to another (D. A. Williams, private communication). Also, of course, the CH microwave lines are much weaker than those of CO.

For diffuse clouds, the CH method gives a smaller rms scatter than the atomic H method and so it is to be preferred. If both are available, it would be appropriate to combine the results, weighted according to the respective rms scatters.

Acknowledgments

We thank Dr S. R. Federman for his comments on a draft of this paper. WBS is grateful to Dr A. E. Wright for suggestions and discussions about the detectability of the H$_2$ ultrafine-structure transition.

References


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